

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
1-1 (#1)	-	liquid	100%	n.p.	Severe	Category 2A	Category I	R36	Irritant	Irritant	Cat I	Swanson and Harbell (2000)
1-2 (#2)	-	liquid	100%	n.p.	Mild	Category 2A	Category II	R36	Irritant	Irritant	Cat III	Swanson and Harbell (2000)
1-3 (#3)	-	liquid	100%	n.p.	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Swanson and Harbell (2000)
1-Naphthalene acetic acid	86-87-3	solid	20%	96	Very Severe	Category 1	Category I	SCNM	Irritant	Irritant	Cat II	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	solid	20%	95	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
1-Nitropropane	108-03-2	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
1-Phenyl-3-pyrazolidone	92-43-3	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
1,2,3-Trichloropropane	96-18-4	liquid	100%	n.p.	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
1,2,4-Trimethylbenzene	95-63-6	liquid	100%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
2-4 (#4)	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Swanson and Harbell (2000)
2-7 (#7)	-	liquid	100%	n.p.	Moderate	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Swanson and Harbell (2000)
2-8 (#8)	-	liquid	100%	n.p.	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat II	Swanson and Harbell (2000)
2-Aminophenol	95-55-6	solid	20%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
2-Chloro-2,4,4-trimethylpentane	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Irritant	Irritant	Cat III	Bailey et al. (2004)
2-Ethoxyethanol	110-80-5	liquid	100%	n.p.	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat I	Gautheron et al. (1994)
2-Ethyl-1-hexanol	104-76-7	liquid	100%	99	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
2-Mercaptopyrimidine	1450-85-7	solid	20%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
2-Methoxyethanol	109-86-4	liquid	100%	n.p.	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
2,2-Dimethylbutanoic acid	595-37-9	liquid	100%	96	Very Severe	SCNM	Category I	SCNM	Irritant	Irritant	Cat I	Balls et al. (1995)
2,4-Dichloro-5-sulfamoylbenzoic acid	2736-23-4	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)

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2,4-Pentanedione	123-54-6	liquid	100%	n.p.	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
2,5-Dimethylhexanediol	110-03-2	solid	20%	99.5	Mild	Category I	Category I	R41	Irritant	Irritant	Cat III	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	liquid	100%	99	Mild	Category 2A	Category II	SCNM	Irritant	Irritant	Cat III	Balls et al. (1995)
3-Glycidioxypropyltrimethoxysilane	2530-83-8	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	solid	20%	95	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Southee (1998)
5-Ethylidene-2-norbornene	16219-75-3	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant			Cat III	Bailey et al. (2004)
A		n.p. ¹²	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AB		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AC		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Acetone	67-64-1	liquid	100%	99	Very Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat I	Balls et al. (1995)
AD		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AE		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat II	AMCP BRD
AF		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
AG		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Inconclusive	Cat I	AMCP BRD
AH		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	SCNM	SCNM	Cat I	AMCP BRD
AI		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AJ		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AK		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AL		n.p.	n.p.	n.p.	Cat I	Category 2A	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Alkyl phosphoric acid ester/amine	-	liquid	100%	n.p.	Severe	Category I	SCNM	R41	Irritant	Irritant	Cat I	Bailey et al. (2004)

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All Purpose Cleaner (#5)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
All Purpose Cleaner (#7)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Allyl alcohol	107-18-6	liquid	100%	n.p.	Severe	Category 2A	Category III	R36	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Aluminum hydroxide	21645-51-2	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
AM		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Ammonium nitrate	6484-52-2	solid	20%	>99.9	Mild	Category 2B	Category III	R36	Irritant	Irritant	Cat III	Balls et al. (1995)
Ammonium nitrate	6484-52-2	n.p.	100%	n.p.	Mild	Category 2B	Category III	R36	Irritant	Irritant	Mild	Southee (1998)
AN		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Not labeled	Not labeled	Cat I	AMCP BRD
Anthracene	120-12-7	solid	20%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
AO		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AP		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AQ		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AR		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Aromatic hydrocarbon #1	-	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Aryl phosphonates	-	liquid	100%	n.p.	Moderate	Category 2B	SCNM	SCNM	Irritant	Irritant	Cat II	Bailey et al. (2004)
AS		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AT		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AU		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AV		n.p.	n.p.	n.p.	Cat I	Category I	Category I	n.p.	SCNM	SCNM	Cat I	AMCP BRD
AW		n.p.	n.p.	n.p.	Cat II	Category I	Category I	n.p.	Irritant	Irritant	Cat II	AMCP BRD

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AX		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
AY		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
B		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Bathroom Cleaner (#6)	-	liquid	100%	n.p.	Severe	SCNM	Category III	Nonirritant	Irritant	Irritant	Cat I	Swanson et al. (1995)
BB		n.p.	n.p.	n.p.	Cat III	SCNM	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
BD		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat III	AMCP BRD
BE		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Irritant	Inconclusive	Cat III	AMCP BRD
Benchmark-Group 1 (#12)	-	liquid	100%	n.p.	Severe	Category 2A	Category I	R36	Irritant	Irritant	Cat II	Swanson and Harbell (2000)
Benchmark-Group 2 (#13)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat II	Swanson and Harbell (2000)
Benzalkonium chloride (1 %)	8001-54-5	liquid	1%	98	Very Severe	Category 1	Category II	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	liquid	10%	98	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Benzalkonium chloride (100%)	8001-54-5	liquid	10%	n.p.	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Southee (1998)
Benzalkonium chloride (5%)	8001-54-5	liquid	5%	98	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Benzethonium chloride	121-54-0	surfactant	10%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Benzoyl-L-tartaric acid	2743-38-6	solid	20%		Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Betaine monohydrate	590-47-6	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Gautheron et al. (1994)
BF		n.p.	n.p.	n.p.	Cat I	Category 2A	Category III	n.p.	Irritant	Irritant	Cat II	AMCP BRD
BJ		n.p.	n.p.	n.p.	Cat I	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat I	AMCP BRD
BJ		n.p.	n.p.	n.p.	Cat II	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat II	AMCP BRD
BK		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat III	AMCP BRD
BL		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD

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BM		n.p.	n.p.	n.p.	Cat II	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat II	AMCP BRD
BN		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
BP		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
BQ		n.p.	n.p.	n.p.	Cat II	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat II	AMCP BRD
BRIJ-35	9002-92-0	surfactant	10%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
Butyl acetate	123-86-4	liquid	100%	99	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat II	Balls et al. (1995)
Butyl cellulose	111-76-2	liquid	100%	n.p.	Very Severe	Category I	Category II	R41	Irritant	Irritant	Cat I	Southee (1998)
Butyrolactone	96-48-0	liquid	100%	n.p.	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Gautheron et al. (1994)
C		n.p.	n.p.	n.p.	Cat II	Category I	Category I	n.p.	Irritant	Irritant	Cat II	AMCP BRD
Captan 90 concentrate	133-06-2	solid	20%	90	Moderate	Category I	Category I	R41	Irritant	Irritant	Cat II	Balls et al. (1995)
Carboxylic acid amides	-	solid	100%	n.p.	Moderate	Category I	Category I	R41	Irritant	Irritant	Cat II	Bailey et al. (2004)
Cetylpyridinium bromide (0.1%)	140-72-7	liquid	0.10%	98	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	liquid	10%	98	Very Severe	Category I	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	liquid	6%	98	Severe	Category I	SCNM	R41	Irritant	Irritant	Cat II	Balls et al. (1995)
CG		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
CH		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Irritant	Inconclusive	Cat III	AMCP BRD
Chlorhexidine	55-56-1	solid	20%	n.p.	Very Severe	Category I	SCNM	SCNM	Irritant	Irritant	Cat I	Balls et al. (1995)
Clarified slurry oil	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Cleaner/Degreaser (#13)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Cutting fluid (conc.) #1	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Cutting fluid (conc.) #2	-	liquid	100%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Bailey et al. (2004)

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Cyclohexanol	108-93-0	liquid	100%	97	Moderate	Category 1	Category I	R41	Irritant	Irritant	Cat II	Balls et al. (1995)
Cyclohexanone	108-94-1	liquid	100%	n.p.	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat I	Gautheron et al. (1994)
D		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Degreaser (#16)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Deoxycholic acid, sodium salt	302-95-4	surfactant	10%	n.p.	Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Diacetone alcohol	123-42-2	liquid	100%	n.p.	Moderate	SCNM	SCNM	SCNM	Irritant	Irritant	Cat II	Gautheron et al. (1994)
Dibenzoyl-L-tartaric acid	2743-38-6	solid	20%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Dibenzyl phosphate	1623-08-1	solid	20%	99	Very Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat I	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	liquid	100%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
Dimethylbiguanide	657-24-9	solid	20%	n.p.	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
DL-Glutamic acid	19285-83-7	solid	20%	n.p.	Nonirritant	SCNM	SCNM	SCNM	Irritant	Inconclusive	Cat III	Gautheron et al. (1994)
E		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	SCNM	SCNM	Cat I	AMCP BRD
EDTA, di-potassium salt	25102-12-9	solid	20%	n.p.	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
EF		n.p.	n.p.	n.p.	Cat I	Category 2A	Category II	n.p.	Irritant	Irritant	Cat I	AMCP BRD
EG		n.p.	n.p.	n.p.	Cat I	Category 2A	Category II	n.p.	Irritant	Irritant	Cat II	AMCP BRD
Ethanol	64-17-5	liquid	100%	n.p.	Severe	Category 2A	Category III	Nonirritant	Irritant	Irritant	Cat I	Balls et al. (1995)
Ethanol	64-17-5	liquid	100%	n.p.	Severe	SCNM	Category II	Nonirritant	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Ethanol	64-17-5	liquid	100%	n.p.	Moderate	Category 2A	Category III	Nonirritant	Irritant	Irritant	Cat II	Southee (1998)
Ethyl acetate	141-78-6	liquid	100%	99	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Balls et al. (1995)
Ethyl acetoacetate	141-97-9	liquid	100%	n.p.	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
Ethyl trimethyl acetate	3938-95-2	liquid	100%	99	Mild	Nonirritant	Category III	Nonirritant	Not labeled	Not labeled	Cat III	Balls et al. (1995)

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Ethyl-2-methylacetoacetate	609-14-3	liquid	100%	97	Mild	Category 2B	Category III	Nonirritant	Irritant	Irritant	Cat III	Balls et al. (1995)
Ethylhexyl acid phosphate ester	-	liquid	100%	n.p.	Severe	Category 1	SCNM	R41	Irritant	Irritant	Cat I	Bailey et al. (2004)
F		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Floor Cleaner (#10)	-	liquid	100%	n.p.	Severe						Cat II	Swanson et al. (1995)
Floor Cleaner (#2)	-	liquid	100%	n.p.	Nonirritant						Cat III	Swanson et al. (1995)
Floor Stripper (#14)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Floor Stripper (#17)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Floor Stripper (#18)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Fomesafen	72128-02-0	solid	20%	97.5	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Balls et al. (1995)
Furan	110-00-9	liquid	100%	n.p.	Severe	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
G		n.p.	n.p.	n.p.	Cat I	Category 1	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
gamma-Butyrolactone	96-48-0	liquid	100%	>99	Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
General Cleaner (#11)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
General Cleaner (#12)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Glass Cleaner (#19)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Gluconolactone	90-80-2	solid	20%	n.p.	Severe	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat I	Gautheron et al. (1994)
Glycerol	56-81-5	liquid	100%	>99.5	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Balls et al. (1995)
Glycerol	56-81-5	liquid	100%	>99.5	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Nonirritant	Southee (1998)
H		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category II	n.p.	Irritant	Irritant	Cat III	AMCP BRD
Heavy Duty Cleaner (#15)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Heavy Duty Cleaner/Degreaser (#9)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	Moderate	Category 1	Category I	R41	Irritant	Irritant	Cat II	Gautheron et al. (1994)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
Hexadecyltrimethylammonium bromide	57-09-0	surfactant	10%	n.p.	Moderate	Category 1	Category I	R41	Irritant	Irritant	Cat II	Southee (1998)
Hexane	110-54-3	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
I		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Imidazole	288-32-4	solid	20%	99	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Imidazole	288-32-4	solid	20%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant		Gautheron et al. (1994)
Imidazole	288-32-4	solid	20%	n.p.	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Very Severe	Southee (1998)
Iminodibenzyl	494-19-9	solid	20%	n.p.	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
Isobutanol	78-83-1	liquid	100%	99.9	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
Isopropanol	67-63-0	liquid	100%	99.9	Severe	Category 2A	Category III	SCNM	Irritant	Irritant	Cat II	Balls et al. (1995)
J		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat III	AMCP BRD
K		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
L		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category III	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
L-Aspartic acid	70-47-3	solid	20%	100	Nonirritant	SCNM	SCNM	SCNM	Irritant	Irritant	Cat III	Balls et al. (1995)
Laurylsulfobetaine	14933-08-5	surfactant	10%	n.p.	Severe	SCNM	SCNM	SCNM	Irritant	Irritant	Cat I	Gautheron et al. (1994)
M		n.p.	n.p.	n.p.	Cat I	Nonirritant	Category III	n.p.	Irritant	Irritant	Cat II	AMCP BRD
Magnesium carbonate	56378-72-4	solid	20%	n.p.	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
Maneb	12427-38-2	solid	20%	90	Mild	SCNM	Category III	SCNM	Irritant	Irritant	Cat II	Balls et al. (1995)
Meat Room Degreaser (#3)	-	liquid	100%	n.p.	Severe						Cat I	Swanson et al. (1995)
Metal Cleaner (#20)	-	liquid	100%	n.p.	Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Swanson et al. (1995)
Methanol	67-56-1	liquid	100%	n.p.	Severe	Nonirritant	Category II	Nonirritant	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Methyl acetate	79-20-9	liquid	100%	98	Moderate	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)

Comparison of In Vivo and In Vitro Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
Methyl cyanoacetate	105-34-0	liquid	100%	99	Mild	Category 2A	Category II	R36	Irritant	Irritant	Cat III	Balls et al. (1995)
Methyl cyclopentadiene dimer	-	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Methyl ethyl ketone	78-93-3	liquid	100%	99	Severe	Category 2A	Category III	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	liquid	100%	99	Severe	Category 2B	Category III	R36	Irritant	Irritant	Cat II	Southee (1998)
Methyl isobutyl ketone	108-10-1	liquid	100%	98	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Balls et al. (1995)
Methylcyclopentane	96-37-7	liquid	100%	>99	Nonirritant	Nonirritant	Category III	Nonirritant	Not labeled	Not labeled	Cat III	Balls et al. (1995)
Methylisobutyl ketone	108-10-1	liquid	100%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Gautheron et al. (1994)
MYRJ-45	-	surfactant	10%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
N		n.p.	n.p.	n.p.	Cat I	Nonirritant	Category III	n.p.	Irritant	Inconclusive	Cat I	AMCP BRD
n-Hexanol	111-27-3	liquid	100%	98	Severe/Very Severe	Category 2A	Category II	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
N-Lauroylsarcosine, sodium salt	7631-98-3	surfactant	10%	n.p.	Moderate	Category 2B	Category III	Nonirritant	Irritant	Irritant	Cat II	Gautheron et al. (1994)
n-Octanol	111-87-5	liquid	100%	>99	Moderate	Category 2B	Category III	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
O		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Octanol	111-87-5	liquid	100%	n.p.	Moderate	Category 2B	Category III	R36	Irritant	Irritant	Cat II	Gautheron et al. (1994)
P		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Parafluoraniiline	371-40-4	liquid	100%	99	Moderate	SCNM	SCNM	SCNM	Irritant	Irritant	Cat II	Balls et al. (1995)
Parafluoraniiline	371-40-4	liquid	100%	99	Moderate	SCNM	SCNM	SCNM	Irritant	Irritant	Cat II	Southee (1998)
Petroleum ether	8032-32-4	liquid	100%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Gautheron et al. (1994)
Petroleum wax	-	solid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Phenylbutazone	50-33-9	solid	20%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
Polyalkenylsuccinate ester/amine s	-	liquid	100%	n.p.	Nonirritant	SCNM	Category III	SCNM	Irritant	Irritant	Cat III	Bailey et al. (2004)

Comparison of In Vivo and In Vitro Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
Polyethylene glycol 400	25322-68-3	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Balls et al. (1995)
Pot and Pan Cleaner (#8)	-	liquid	100%	n.p.	Nonirritant						Cat III	Swanson et al. (1995)
Potassium cyanate	590-28-3	solid	20%	97	Mild	SCNM	SCNM	SCNM	Irritant	Irritant	Cat III	Balls et al. (1995)
Process oil	-	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Bailey et al. (2004)
Promethazine hydrochloride	58-33-3	solid	20%	98	Severe	Category I	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	solid	20%	n.p.	Severe	Category I	Category I	R41	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
Propyl-4-hydroxybenzoate	94-13-3	solid	20%	100	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Southee (1998)
Pyridine	110-86-1	liquid	100%	>99.9	Severe	Category I	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Pyridine	110-86-1	liquid	100%	n.p.	Severe	Category I	Category I	R41	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Q		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Quinacrine	69-05-6	solid	20%	n.p.	Mild	Category I	Category I	R41	Irritant	Irritant	Cat III	Balls et al. (1995)
Quinacrine	69-05-6	solid	20%	n.p.	Moderate	Category I	Category I	R41	Irritant	Irritant	Cat III	Gautheron et al. (1994)
R		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
S		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Sodium hydroxide (1%)	1310-73-2	liquid	1%	reagent grade	Very Severe	Category 2B	Category III	R36	Irritant	Irritant	Cat I	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	reagent grade	Severe	Category I	Category I	R41	SCNM	SCNM	Cat I	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	liquid	10%	n.p.	Very Severe	Category I	Category I	R41	SCNM	SCNM	Cat I	Southee (1998)
Sodium lauryl sulfate (15 %)	151-21-3	liquid	15%	98	Mild	Category I	Category I	R36	Irritant	Irritant	Cat II	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	liquid	15%	98	Mild	Category I	Category I	SCNM	Irritant	Irritant	Cat III	Southee (1998)
Sodium lauryl sulfate (3 %)	151-21-3	liquid	3%	98	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Balls et al. (1995)

Comparison of *In Vivo* and *In Vitro* Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
Sodium oxalate	62-76-0	solid	20%	>99	Mild	Category 1	Category I	R41	Irritant	Irritant	Cat III	Balls et al. (1995)
Sodium oxalate	62-76-0	solid	20%	n.p.	Mild	Category 1	Category I	R41	Irritant	Irritant		Gautheron et al. (1994)
Sodium oxalate	62-76-0	solid	20%	99	Nonirritant	Category 1	Category I	R41	Irritant	Irritant	Cat III	Southee (1998)
Sodium perborate	10486-00-7	solid	20%	98.6	Very Severe	Category 1	Category I	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
T		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	97	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	solid	20%	n.p.	Mild	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat III	Gautheron et al. (1994)
Thiadiazole alkyl derivative	-	liquid	100%	n.p.	Moderate	SCNM	Category III	SCNM	Irritant	Irritant	Cat III	Bailey et al. (2004)
Thiourea	62-56-6	solid	20%	>99	Severe	SCNM	SCNM	SCNM	Irritant	Irritant	Cat I	Balls et al. (1995)
Thiourea	62-56-6	solid	20%	n.p.	Severe	SCNM	SCNM	SCNM	Irritant	Irritant	Cat I	Gautheron et al. (1994)
Toilet Bowl Cleaner (#1)	-	liquid	100%	n.p.	Mild	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Swanson et al. (1995)
Toilet Bowl Cleaner (#4)	-	liquid	100%	n.p.	Mild	Nonirritant	SCNM	Nonirritant	Irritant	Inconclusive	Cat III	Swanson et al. (1995)
Toluene	108-88-3	liquid	100%	99	Moderate	Nonirritant	Category III	Nonirritant	Irritant	Irritant	Cat II	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	liquid	3%	reagent grade	Severe/Very Severe	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat I	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	liquid	30%	reagent grade	Very Severe	Category 1	Category I	R41	SCNM	SCNM	Cat I	Balls et al. (1995)
Triethanolamine	102-71-6	liquid	100%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
Triton X-100 (10%)	9002-93-1	liquid	10%	98	Severe/Very Severe	Category 1	Category II	R41	Irritant	Irritant	Cat I	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	liquid	5%	98	Severe	Category 2A	Category III	R36	Irritant	Irritant	Cat I	Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	liquid	5%	98	Mild	Category 2B	Category III	R36	Irritant	Irritant	Cat III	Southee (1998)
Triton X-155	9010-44-0	surfactant	10%	n.p.	Nonirritant	Nonirritant	Category IV	Nonirritant	Not labeled	Not labeled	Cat III	Gautheron et al. (1994)
Tween 20	9005-64-5	liquid	n.p.	98	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Cat III	Balls et al. (1995)

Comparison of In Vivo and In Vitro Ocular Irritancy Classifications: Sorted by Substance

Substance	CASRN	Form Tested	Concentration Tested	Purity (%)	<i>In Vitro</i> Consensus Classification Severe \geq 55.1 ¹	<i>In Vivo</i> GHS ^{2,3}	<i>In Vivo</i> EPA ^{4,5}	<i>In Vivo</i> EU ^{6,7}	FHSA-20% ⁸	FHSA-67% ⁹	<i>In Vitro</i> Consensus Classification Severe \geq 75 ¹	Reference
Tween 20	9005-64-5	liquid	100%	98	Nonirritant	Nonirritant	Category III	Nonirritant	Irritant	Inconclusive	Nonirritant	Southee (1998)
U		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
V		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
W		n.p.	n.p.	n.p.	Cat III	Nonirritant	Category IV	n.p.	Not labeled	Not labeled	Cat III	AMCP BRD
X		n.p.	n.p.	n.p.	Cat I	Category 2A	Category I	n.p.	Irritant	Irritant	Cat I	AMCP BRD
Y		n.p.	n.p.	n.p.	Cat I	Category 2A	Category II	n.p.	Irritant	Irritant	Cat II	AMCP BRD
Z		n.p.	n.p.	n.p.	Cat II	Category 2A	Category II	n.p.	Irritant	Irritant	Cat II	AMCP BRD

Abbreviations: CASRN = Chemical Abstract Services Registry Number; SCNM = study criteria not met; n.p. = not provided

¹ Consensus classification represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls

² GHS=Globally Harmonized System (UN 2007)

³ Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

⁴ EPA = U.S. Environmental Protection Agency (EPA 2003a).

⁵ Toxicity Category I for the Primary Eye Irritation Study = corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = corneal involvement or irritation clearing in 8-21 days; Category III = corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

⁶ EU=European Union (EU 2001).

⁷ Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

⁸ FHSA=Federal Hazardous Substance Act (2005). FHSA-20% is based on the proportion of positive animals needed to identify a substance as an irritant using the FHSA sequential testing strategy, where 20% of the animals need to demonstrate a positive response for a substance to be identified as an irritant. A substance tested using 3 to 6 animals would not be labeled if \leq 1/6 animals were positive based on the FHSA criteria. The substance would be labeled as an irritant if there were \geq 1 positive animal in a 3 to 5 animal test or \geq 2 positive animals in a 6 animal test.

⁹ FHSA=Federal Hazardous Substances Act (2005). FHSA-67% is based on the proportion of positive animals needed to identify a substance as an irritant using the "first test" of the FHSA sequential testing strategy, where 67% of the animals need to demonstrate a positive response for a substance to be identified as an irritant. A substance tested using 3 to 6 animals would not be labeled if \leq 1/6 animals were positive based on the FHSA criteria. The substance would be labeled as an irritant if there were \geq 2/3, 3/4, 4/5, or 4/6 positive animals. If 1/3, 1/4, 2/4, 1/5, 2/5, 3/5, 2/6, or 3/6 animals were positive, further testing would be required.